Materials and Equipment:

Solar Cell Materials

	Cell Size (Converted Units)	Materials	Layer Thickness (Raw Units)
Trial 1	Substrate – 100 nm	Glass	1e-08
	Width = 100 nm	PEDOT:PSS	1e-08
	Length = 400 nm	PBDB-T:ITIC	1e-07
		Aluminum	1e-08
Trial 2	Substrate – 175 nm	Glass	1e-08
	Width = 100 nm	PEDOT:PSS	1e-08
	Length = 475 nm	PBDB-T:ITIC	1.75e-7
		Aluminum	1e-08
Trial 3	Substrate –250 nm	Glass	1e-08
	Width = 100 nm	PEDOT:PSS	1e-08
	Length = 550 nm	PBDB-T:ITIC	2.5e-7
		Aluminum	1e-08

Solar Cell Simulation & Modelling Tools

- FreeFem Programming Software (Web Version):
  - https://github.com/FreeFem/FreeFem-sources
- OghmaNano Simulation Software (Version 8 was used)
  - https://www.oghma-nano.com/download.php
- Operating System: Windows 10 Professional (Windows Required)
- PC Specs:
  - MSI GeForce RTX 3060 Gaming X12G GeForce RTX 3060 12GB 12 GB Video Card
  - AMD Ryzen 5 5600 3.5GHz 6-Core Processor
  - Corsair Vengeance LPX 32 GB (2 x 16 GB) DDR4-3600 CL18 Memory
  - Full List of Parts: https://ca.pcpartpicker.com/list/ZH2nJM

Database & Other Software

- All optical data was accessed from the Refractive Index Database: https://refractiveindex.info/
- GitHub Repository with all data stored from this project: https://github.com/deweyliang/SF-2023
- Notepad (Predownloaded on most OS') or Notepad++ – recommend for viewing/editing the database files

Procedure:

Part 1: Designing & Creating the Organic Solar Cell Mesh

For simplified and direct access. click on this link to download the mesh designs: https://github.com/deweyliang/SF-2023/tree/main/meshes/mesh%20designs

1) Open this link into a search engine: https://freefem.org/tryit

2) Once redirected to the coding page, select and copy the mesh/s that you want to design: (https://github.com/deweyliang/SF-2023/tree/main/meshes/mesh%20code)

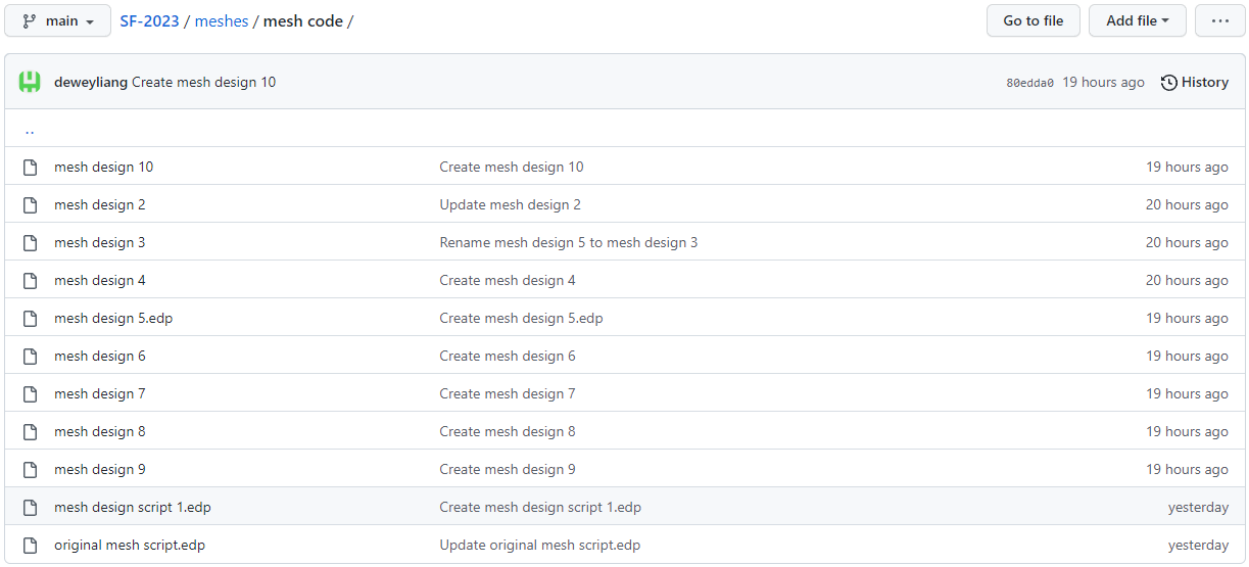

Figure 1: (Old, not updated) version of the mesh repository section

Figure 2: Mesh code

3) In the coding workspace, paste the copied code from the GitHub repository. Click on the "Run" to output the mesh design

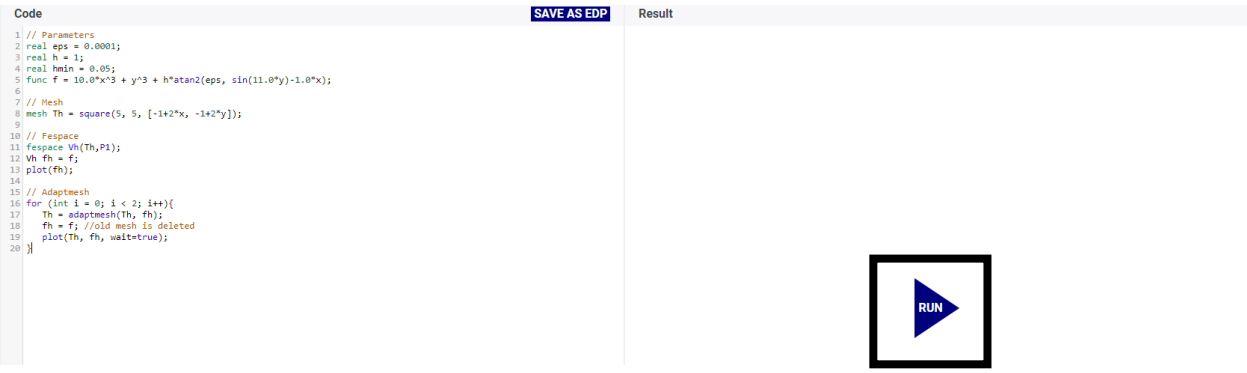

Figure 3: Plugging mesh script into FreeFem

4) If done correctly, an image should appear under “Result”. Right-click and save the image

Software Installation and Starting a New Simulation

1) Install the latest version of the simulation and modelling software (Windows 8+ Only) used in this project: https://www.oghma-nano.com/

2) Once you have opened the software, click on “New Simulation” in the top left corner

3) Open the “Morphology” simulation option and create a new file

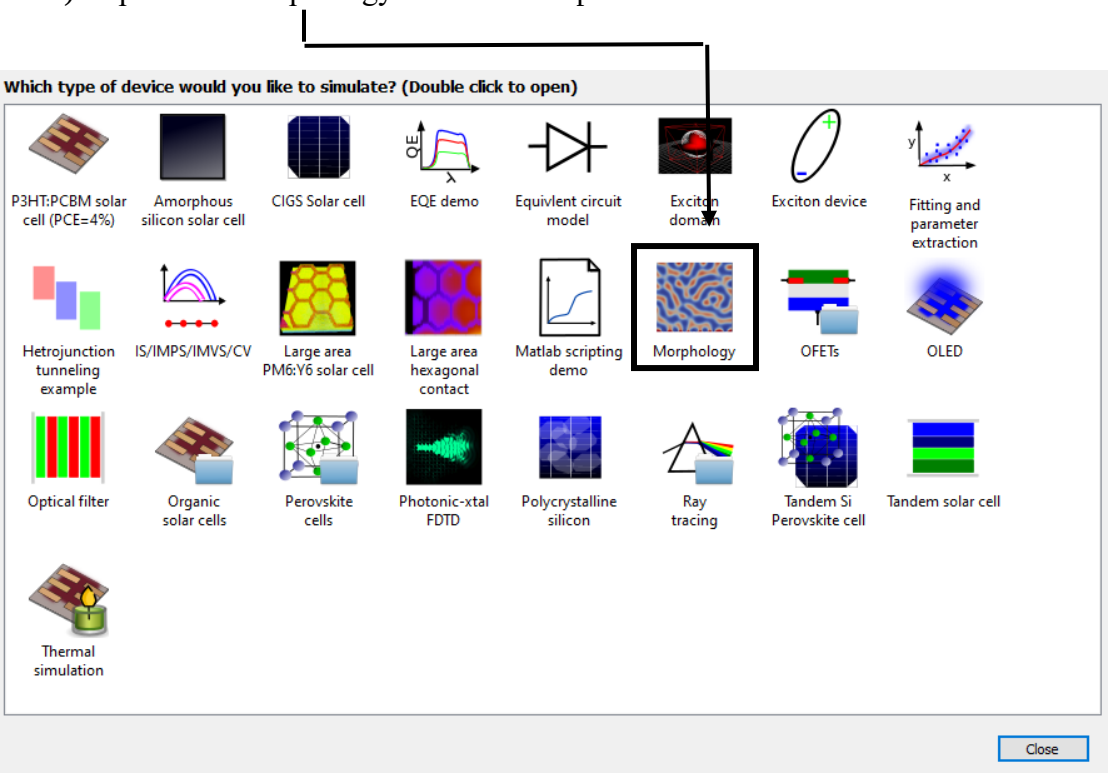

Figure 4: Simulation panel in the software

Importing the Semiconducting Layer Morphology

1) Once inside the simulator, head to “Databases” and click on “Shape Database”

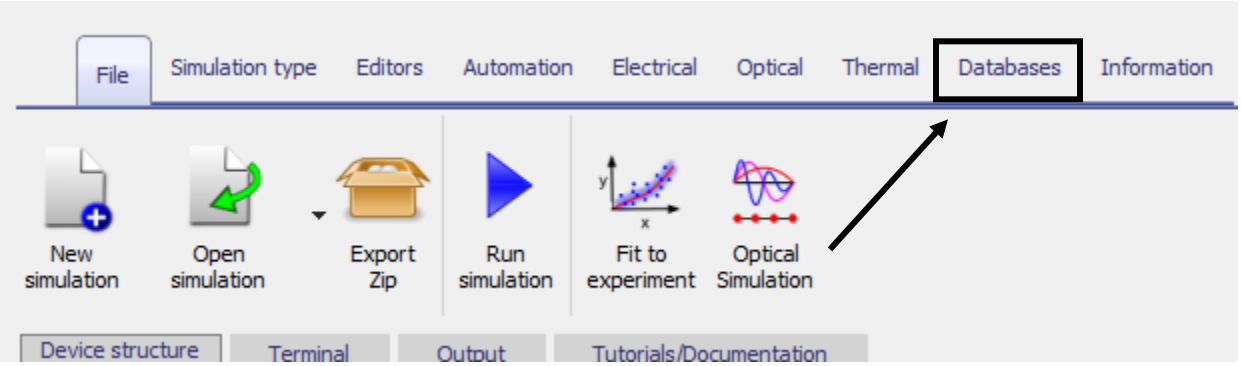

Figure 5: Main Window > Databases

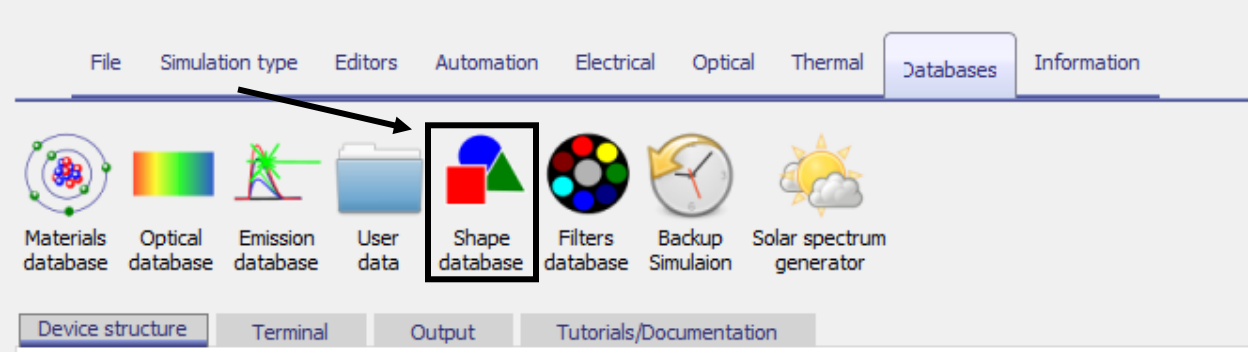

Figure 6: Databases > Shape Database

2) Head over to “Add Shape” and make a recognizable name for the mesh

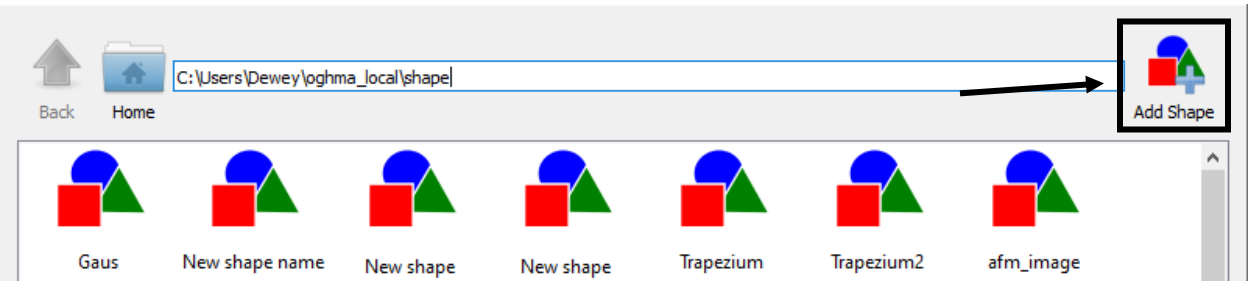

Figure 7: Adding shape into Shape Database

3) After saving the mesh into the local database, scroll until you find the imported mesh and double-click on it

4) Once you have been redirected to another simulation panel, click on “Load New Image”, and import the mesh downloaded from the previous steps

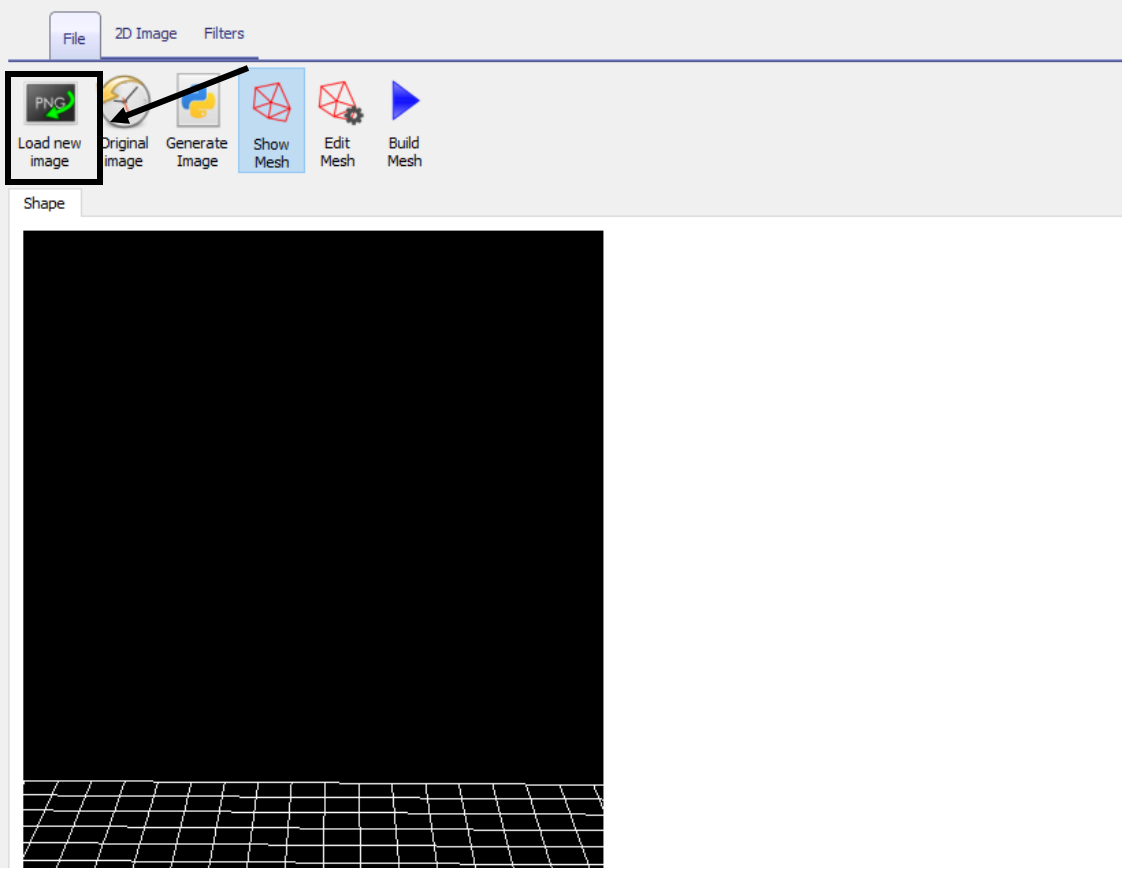

Figure 8: Loading mesh into the simulator

5) If done correctly, an image of the mesh should appear on the right of your screen. Click on “Build Mesh” and wait for the simulation to be completed

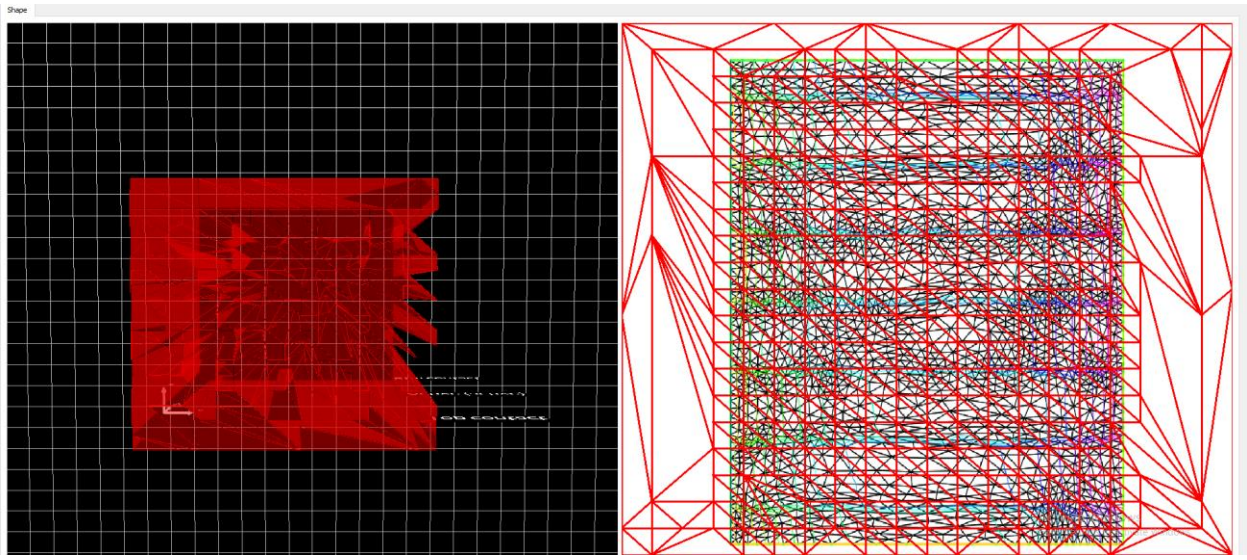

Figure 9: Generated mesh || Mesh design in the triangular-based shape discretizer

Part 2: Extraction & Importation of Optical Data

1) Open this GitHub repository for the optical data: https://github.com/deweyliang/SF-2023/tree/main/data/refractive%20index

2) Select the material that will be imported, and once the file is open, scroll down until you find “tabulated n”. Copy all the data and paste it into a .txt file via Notepad

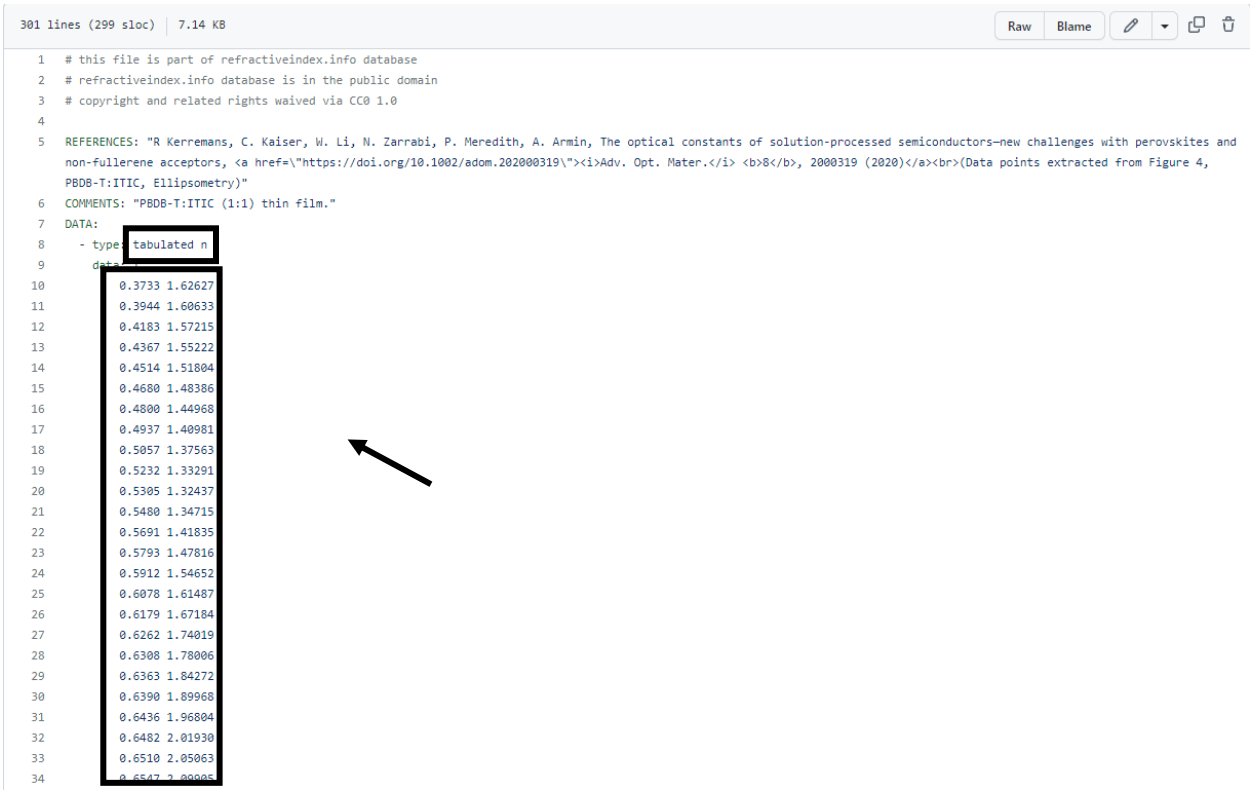

Figure 10: .yml file containing the n and k data for PBDB-T:ITIC

3) Once inside Notepad, click on “File” and save the file. Change the file type from a text document to “All Files” and rename the file and type .dat after the file name.

4) Repeat Steps 2 and 3 but for the “k” value. Save the two files separately.

5) Open the 3D simulator with a solar cell simulation open (for reference, look at Part One of the procedure, under “Importing the Semiconducting Layer Morphology”)

6) Under “Databases”, click on the Materials Database

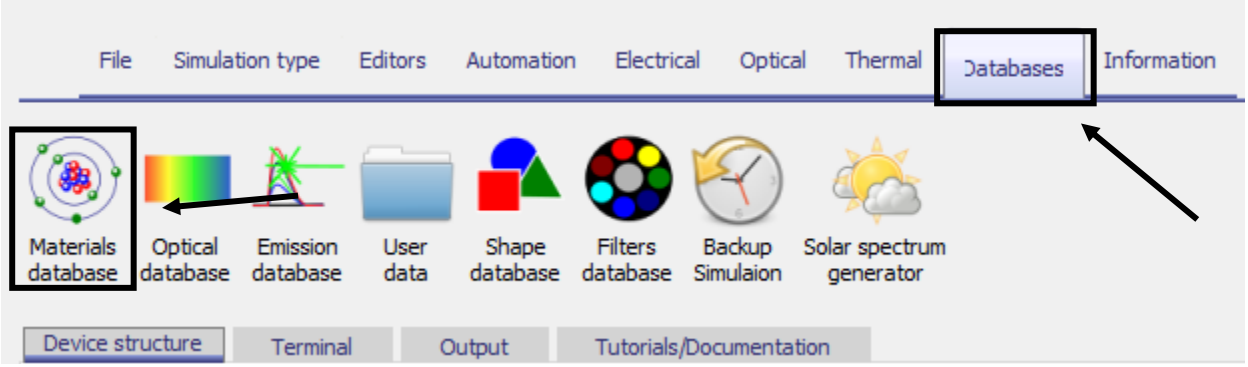

Figure 11: Databases > Materials Database

7) Once inside the materials database, click on "Add Material" and enter a recognizable name for the material

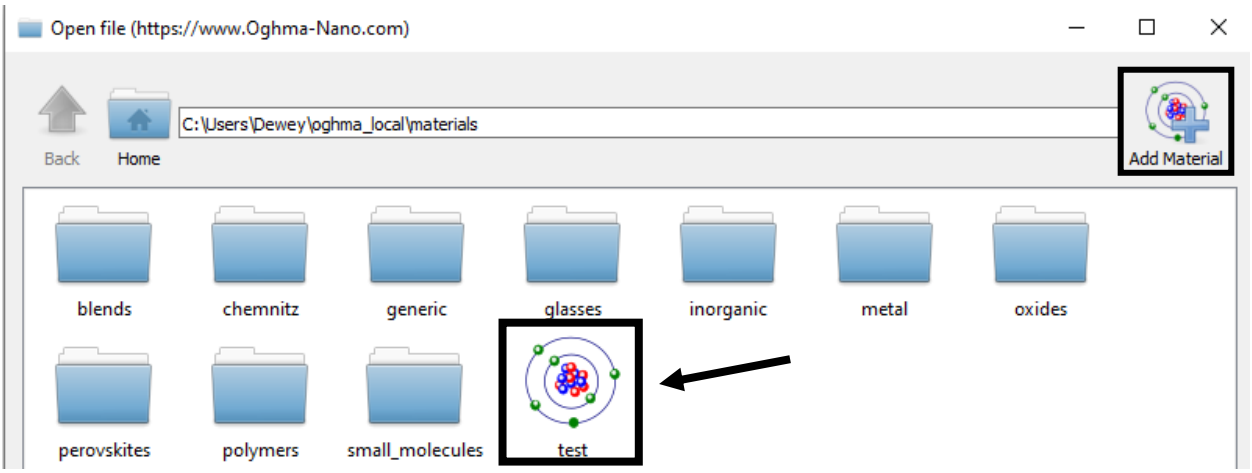

Figure 12: Material output after adding into the database

8) Open the material file created by double-clicking it. Select the "Import from Data" option and import the downloaded data file for the material. The imported tabulated data window should look similar to the images below:

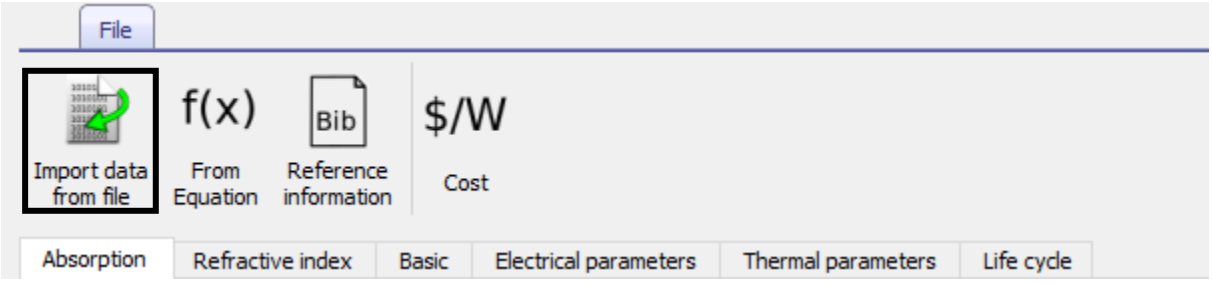

Figure 21: Importing the data file for the "k" value of the selected material

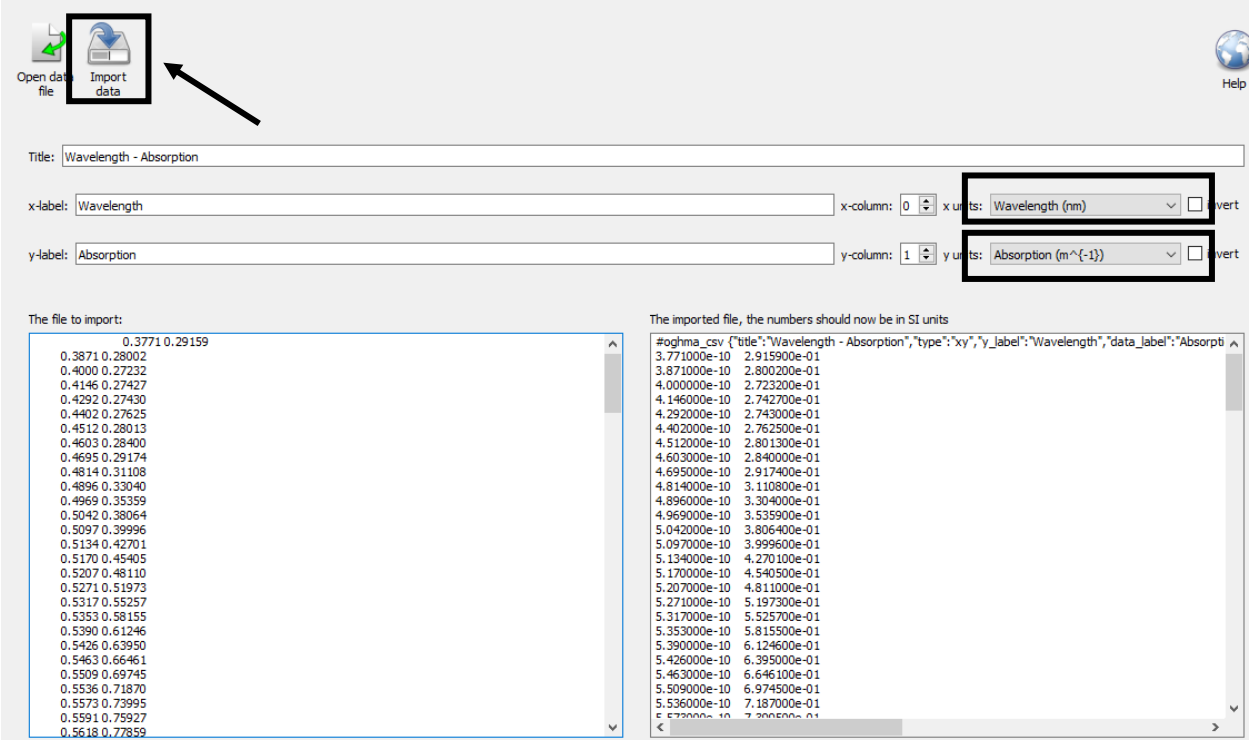

Figure 13: Imported absorption coefficient "k"

9) In the top right corner of the data window, the default values need to be changed - X units to Wavelength (nm) and the y units to Absorption (in meters). Once completed, click on "Import Data."

10) Reopen the material folder that was just imported and under "Refractive index", import the "n" value .dat file from earlier.

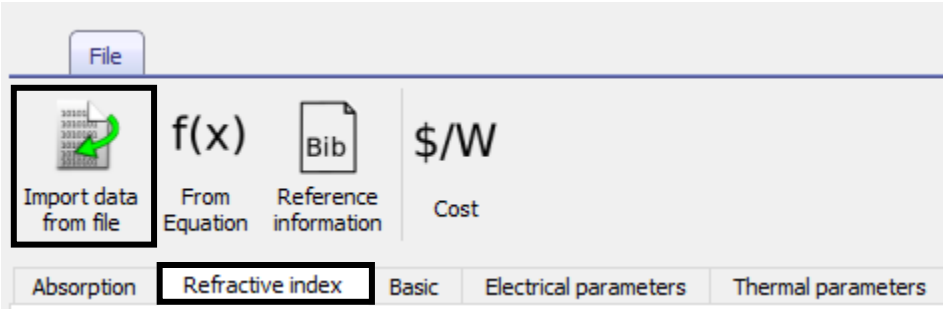

Figure 14: Importing data file for refractive index

11) Now, change the X units to Wavelength (nm) and the Y units to Refractive Index (au) and click on “Import Data”

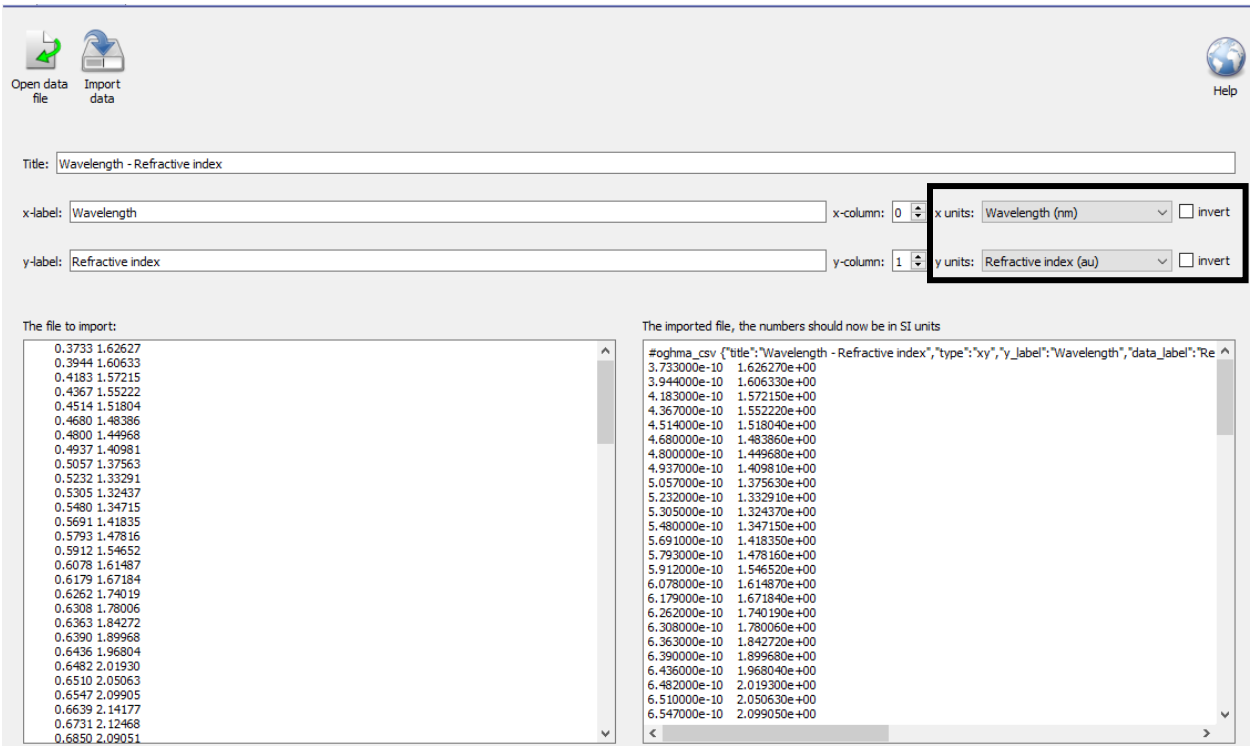

Figure 15: Adjusting units of measurement into SI units

12) Repeat the process until all the materials in the repository (https://github.com/deweyliang/SF-2023/tree/main/data/refractive%20index) have been imported into the database

Part 3: Solar Cell Modelling

Importing Mesh Designs & Morphologies

1) *(Refer back to Part One if in need for clarification, as some steps will be less detailed).* In the 3D simulator, create a new simulation under “Morphology” and under “Shape Database”, add a New Shape

2) Head back to the Shape Database and open the shape file that was created. Click on “Load New Image” and select the mesh design that will be used for experimenting

   (In total, 8 mesh designs were tested, 5 novel mesh designs and 3 other designs which were used to compare results. Open this repository to access and download the meshes: https://github.com/deweyliang/SF-2023/tree/main/meshes/mesh%20designs)

3) Once the mesh has loaded on the right side of the screen, click on “Build Mesh” and wait for it to be complete. Repeat this process until all 10 mesh designs are completed and are in the database as each individual file.

Modelling the Other Solar Cell Components

1) Head to “File” and under “Device Structure”, click on “Layer Editor” and add a layer by clicking on the “+”

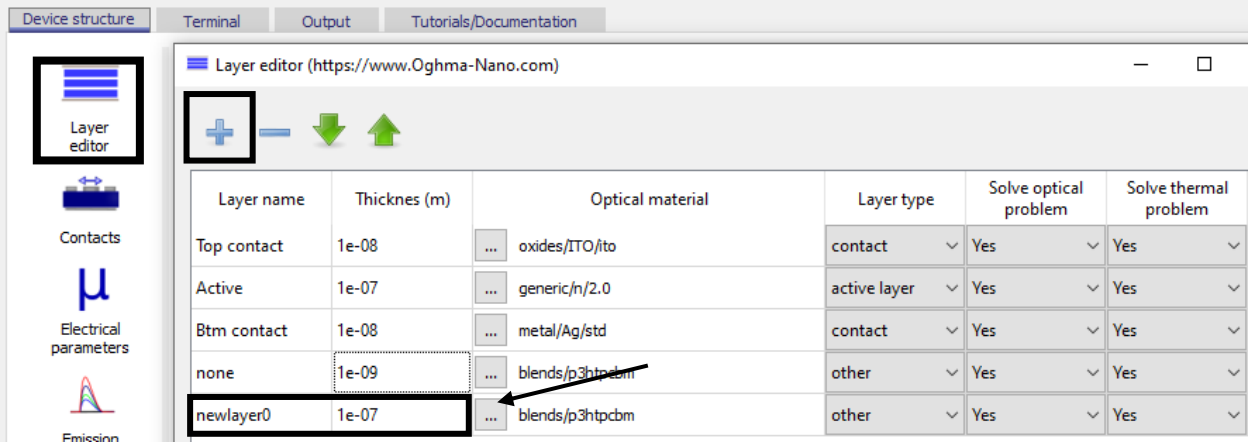

Figure 16: Adding a new layer

2) To change/add materials to each layer, go out into the main overview of the solar cell and right click the layer that will be edited.

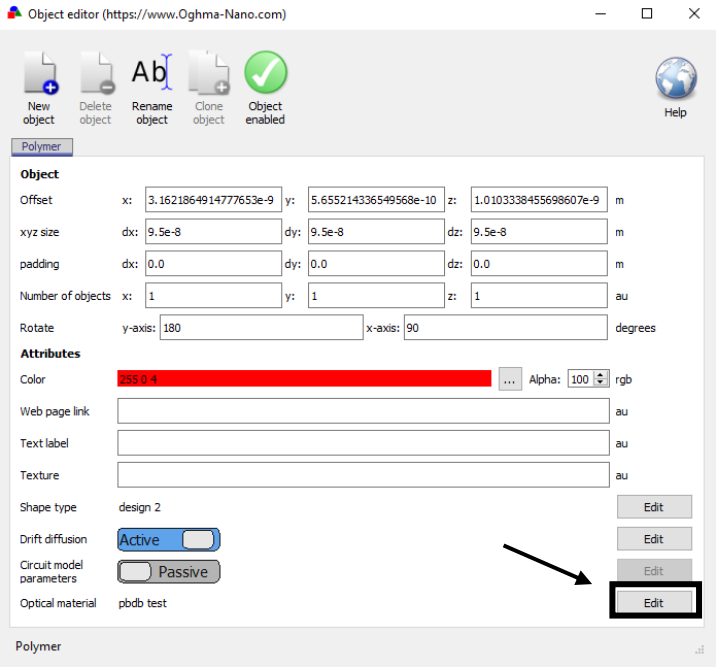

Figure 17: Make sure that drift diffusion is turned on for all materials

3) **This step is optional, but for visualization purposes, each layer was renamed under its respective material by double-clicking on each of the layers under "Layer Name"*

4) For reference, please look at the solar cell material and layer design in "Materials", from descending order, going from top to bottom. Repeat Step 2) until all materials have been imported into the solar cell design

5) When importing PEDOT:PSS, set the material to "Other" under the Layer Type. The other materials should be in the right category.

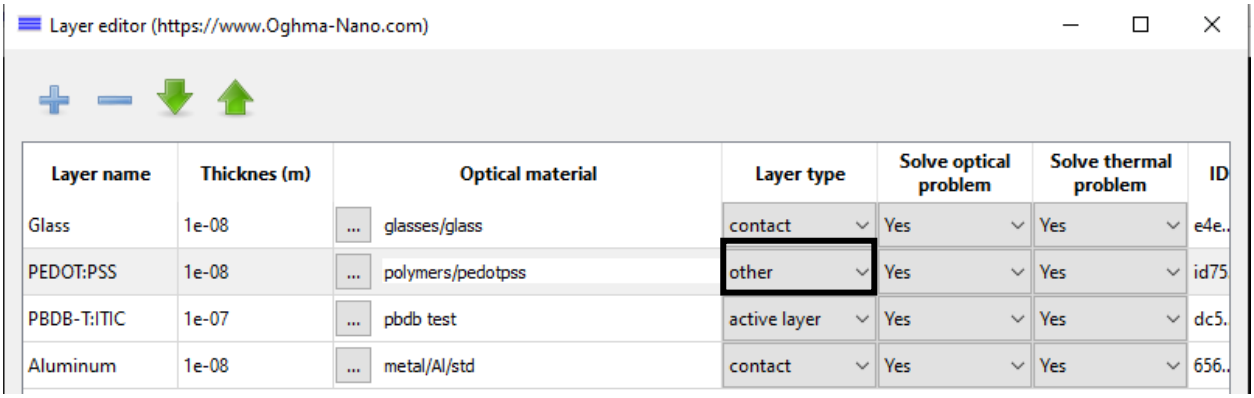

Figure 18: Changing layer type

Part 4: Cell Size & Layer Thickness

Refer back to the materials list for the data needed to for this part of the experiment.

1) Head over to "Electrical" and click on the "Electrical Mesh" icon

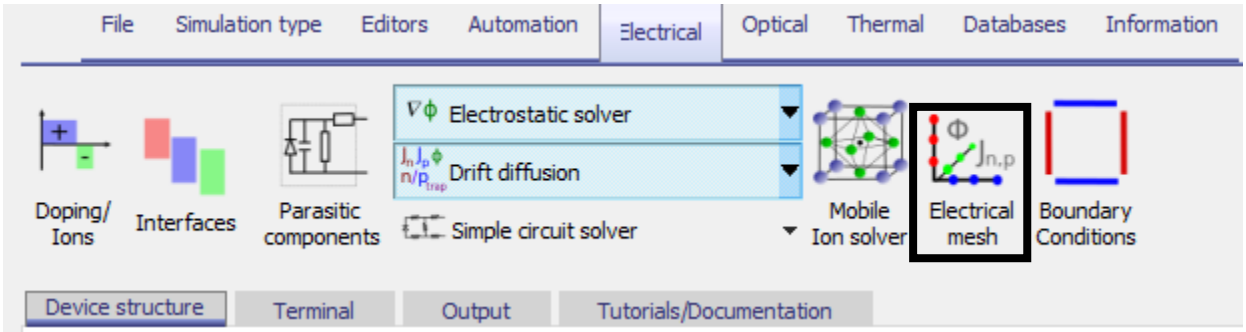

Figure 19: Editing the thickness of the meshes

2) Once inside the panel, make sure only X and Y is on. Click on the "+" and copy the thickness that will be tested. Make sure that the meshes are the same in thickness as well as the other data.

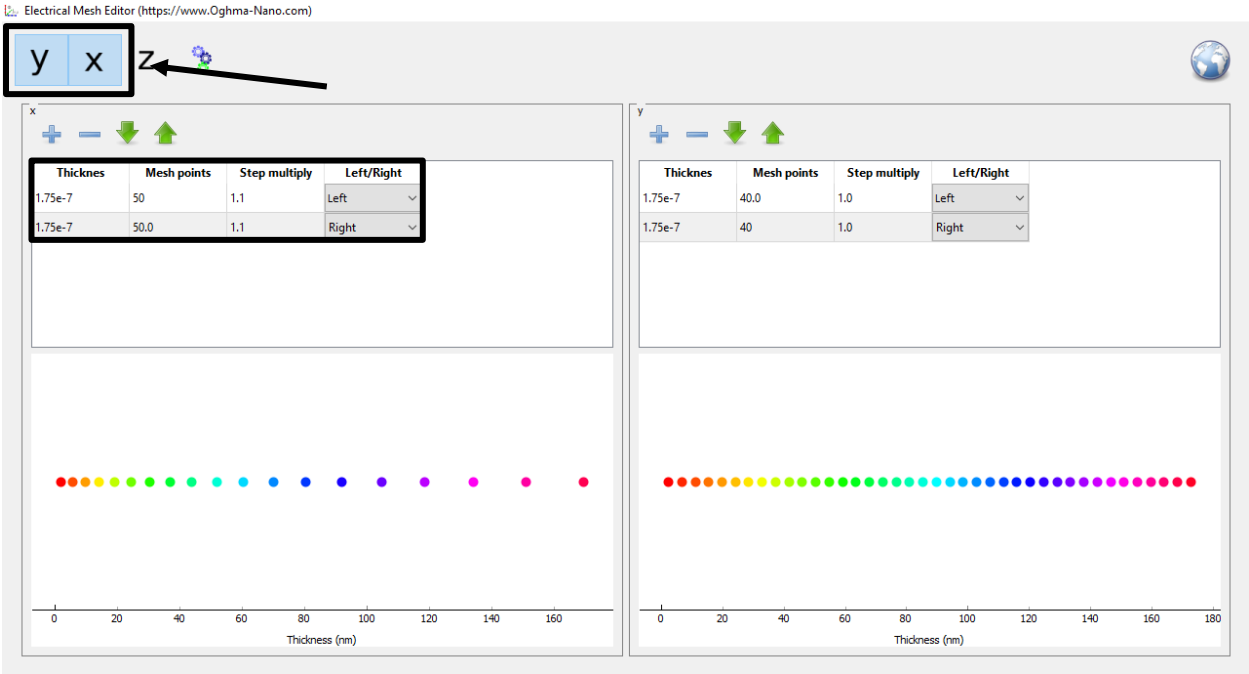

Figure 20: Example with 150 nm

3) Now, go back to the main page and under “Device Structure”, click on “Layer Editor”.

4) Right-click on the mesh and under “Edit”, make the “dy” value the same as the mesh active layer thickness.

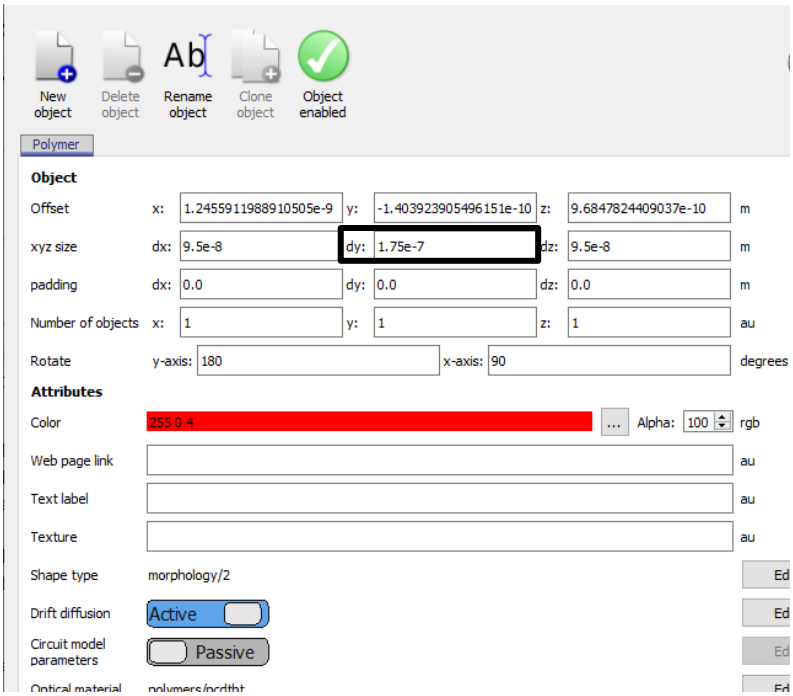

Figure 21: Adjusting size and thickness of cell in layer editor